Role of the transverse field in inverse freezing in the fermionic Ising spin-glass model

S. G. Magalhaes* and C. V. Morais
Universidade Federal de Santa Maria, Santa Maria, Rio Grande do Sul 97105-900, Brazil

F. M. Zimmer
Departamento de Física, Universidade do Estado de Santa Catarina, Joinville, Santa Catarina 89223-100, Brazil

We investigate the inverse freezing in the fermionic Ising spin-glass (FISG) model in a transverse field Γ. The grand canonical potential is calculated in the static approximation, replica symmetry and one-step replica symmetry breaking Parisi scheme. It is argued that the average occupation per site n is strongly affected by Γ. As consequence, the boundary phase is modified and, therefore, the reentrance associated with the inverse freezing is modified too.

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The inverse transitions (melting or freezing), first proposed by Tammann[1], are a class of a quite interesting phase transitions, utterly counterintuitive, in which the ordered phase has more entropy than the disordered one[2]. Despite this apparent unconventional thermodynamics, there is now a list plenty of physical systems in which this sort of transition appears (see Ref. 2 and references therein) including, interestingly, high temperature superconductors.[3] In that sense, the search for theoretical models which contain the necessary ingredients to produce such transitions has become a challenging issue as can be seen in Refs. 2 and 4,5,6. However, much less considerations have been given to models in which quantum effects can also be taken into account.

It should be noticed that there is an important difference among some of the previous mentioned models. For example, in Refs. 2, Schupper and Shnerb show that the Blume-Capel model can present inverse melting since the entropic advantage of the interacting state is introduced in the problem by imposing that the degeneracy parameter $r = k/l \geq 1$, where it is assumed that ± 1 spin states are k-fold degenerated, while 0 spin states are l-fold degenerated. In the Refs. 2 and 4, the classical Ghatak-Sherrington[7] (GS) model has also been proposed to be one of the simplest disordered models to present inverse freezing. Nevertheless, for the GS model, as remarked in Ref. 4, there is no need to enforce the entropic advantage. Thus, the first order boundary of the spin-glass (SG) and/or paramagnetic (PM) transition naturally displays a reentrance. That means it is possible to enter in the SG phase by heating from the PM one. That raises the following questions: is it possible to find other disordered models with inverse freezing but no additional enforcement of the entropic advantage? Would it also be possible to incorporate quantum effects?

It is now well known that the classical GS model has a very close relationship with the fermionic Ising spin-glass (FISG)[8,9] model in the static approximation (SA)[10]. In the FISG model[11,12,13], the spin operators are written by bilinear combination of fermionic creation and destruction operators which act on a space with four eigenstates per site ($|00\rangle, |\uparrow 0\rangle, |0 \downarrow\rangle, |\uparrow\downarrow\rangle$). In particular, the thermodynamics of both models can be exactly mapped by a relationship between the anisotropic constant D and the chemical potential μ of GS and FISG models[8], respectively. Thus, we can expect strong resemblances between the phase diagrams of the two models; particularly, the presence of reentrance in the first order boundary must be emphasized (see, for instance, Ref. 14). Therefore, the FISG model can also be considered one of the models which naturally presents inverse freezing. Actually, the FISG model has been intensively used to study the competition between the SG phase and, for example, superconductivity or Kondo effect (see Refs. 15 and 16 and references therein). Moreover, the FISG has also been used[17] to study the effects of the transverse field Γ on the PM/SG boundary phase within SA. At the half-filling ($\mu = 0$), it has been shown that the increase of Γ strongly changes the FISG thermodynamics since it tends to suppress the SG phase leading the freezing temperature T_f to a quantum critical point (QCP) at Γ_c. Therefore, the FISG model, besides allowing to treat charge and spin at the same level, can be a useful tool to study inverse freezing, particularly, when quantum effects can be included.

The goal of the present paper is to investigate the inverse freezing in the FISG model when spin flipping is induced by a transverse field Γ. It should be remarked that a set of FISG order parameters is composed not only by the usual nondiagonal SG order parameter $q_{\alpha\beta}$ ($\alpha \neq \beta$), but also by the diagonal one $q_{\alpha\alpha}$, which is directly related to the average occupation of fermions per site n[13]. Since Γ affects the behavior of the SG order parameters, we can assume that Γ could have strong influence on n as well. Actually, the behavior of n is determined by a more complicated dependence on Γ than the obvious one given by $q_{\alpha\alpha}$. In that view, the spin flipping produced by Γ can also be considered as a mechanism to change the charge occupation and, hence, to modify the original phase boundary (when $\Gamma = 0$) in the T-μ plane. In this sense, we can probe the robustness of the inverse freezing when quantum effects are present, using what would be, in principle, a controlled external field. In this work, the partition function is obtained within

the Grassmann functional integral formalism[12]. The SG order parameters are calculated within the SA, in the replica symmetry (RS) and one-step replica symmetry breaking (1S-RSB) Parisi scheme. Previous calculations have shown[4] that the position of the first order reentrance has no significant difference when obtained in RS, 1S-RSB or even in the full replica symmetry breaking (FRSB) Parisi scheme[18]. However, to be sure that the first order boundary is not affected by the RS instability when Γ is present, we also obtain the thermodynamics in the 1S-RSB. It should also be highlighted that the use of the SA in the present work can be justified since our main interest is to find the PM-SG phase boundary[19,20]. The FISG model in the presence of transverse field is given by the Hamiltonian

$$\hat{H} = -\sum_{ij} J_{ij} \hat{S}_i^z \hat{S}_j^z - 2\Gamma \sum_i \hat{S}_i^x \quad (1)$$

where the J_{ij} coupling is a Gaussian random variable with mean zero and variance $16J^2$. The spin operators in Eq. (1) are defined as $\hat{S}_i^z = \frac{1}{2}[\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}]$ and $\hat{S}_i^x = \frac{1}{2}[c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}]$ with $\hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ ($\sigma = \uparrow, \downarrow$). We use the procedure introduced in Ref.[17] to obtain the grand canonical potential. Particularly, in the 1S-RSB Parisi scheme, the Grand Canonical Potential is written as

$$\beta\Omega = \frac{(\beta J)^2}{2}[(m-1)q_1^2 - mq_0^2 + \bar{q}^2] - \beta\mu$$
$$- \frac{1}{m}\int Dz \ln\left\{\int Dv[K(z,v)]^m\right\} - \ln 2 \quad (2)$$

where

$$K(z,v) = \cosh(\beta\mu) + \int D\xi \cosh[\sqrt{\Delta(z,v,\xi)}], \quad (3)$$

with $\Delta(z,v,\xi) = [\beta h(z,v,\xi)]^2 + (\beta\Gamma)^2$ and

$$h(z,v,\xi) = J\sqrt{2}(\sqrt{q_0}z + \sqrt{q_1 - q_0}v + \sqrt{\bar{q} - q_1}\xi), \quad (4)$$

where $Dx = dx e^{-x^2/2}/\sqrt{2\pi}$ ($x = z$, v or ξ). In Eqs. (2) and (4), q_0 and q_1 are the 1S-RSB order parameters and $\bar{q} = q_{\alpha\alpha} = \langle S_\alpha^z S_\alpha^z \rangle$ is the diagonal replica spin-spin correlation. The parameters q_0, q_1, $\bar{q}$, and m are given by the extreme condition of the grand canonical potential [Eq. 2]. The RS solution is recovered when $q_0 = q_1 (\equiv q)$ and $m = 0$. In this case, the stability analysis of the RS solution is used in order to locate the tricritical point (T_{t_c}, μ_{t_c}) (Ref. 21) as a function of Γ. Therefore, the condition for all eigenvalues of the Hessian matrix to be non-negative in the PM solution ($q = 0$) is

$$\begin{aligned}\bar{q} &< \frac{1}{\sqrt{2}\beta J} && \text{for } T/J > T_{tc}/J \\ \bar{q} &> \frac{f_\phi(T,\Gamma,\bar{q}) - \sqrt{f_\phi(T,\Gamma,\bar{q}) - 4/(\beta J)^2}}{2} && \text{for } T/J < T_{tc}/J\end{aligned} \quad (5)$$

In Eq. (5), the tricritical temperature T_{tc} is given by

$$T_{tc}/J = \frac{1}{3}\sqrt{2}f_{T_{tc}}(T_{tc}, \Gamma, \bar{q}), \quad (6)$$

with $f_\phi(T, \Gamma, \bar{q})$ defined below,

$$f_\phi(T, \Gamma, \bar{q}) = \frac{\int D\xi \left[\eta_\phi \cosh\sqrt{\Delta_\phi} + \kappa_\phi \sinh\sqrt{\Delta_\phi}\right]}{\int D\xi \left((\bar{h}_\phi^2/\bar{\Delta}_\phi)\cosh\sqrt{\Delta_\phi} + (\beta\Gamma)^2/\bar{\Delta}_\phi^{3/2}\right)} \quad (7)$$

where

$$\begin{aligned}\eta_\phi &= \left\{\bar{h}_\phi^4 + 3(\beta\Gamma)^2\left[1 - 5(\bar{h}_\phi^2/\bar{\Delta}_\phi)\right]\right\}/\bar{\Delta}_\phi^2 \\ \kappa_\phi &= 3(\beta J)^2\left[2\bar{h}_\phi^2 - 1 + 5(\bar{h}_\phi^2/\bar{\Delta}_\phi)\right]/\bar{\Delta}_\phi^{5/2},\end{aligned} \quad (8)$$

and

$$\bar{\Delta}_\phi = \bar{h}_\phi^2 + (\beta\Gamma)^2, \quad \bar{h}_\phi = \beta J\sqrt{2\bar{q}}\xi. \quad (9)$$

In Eq. (6), $f_{T_{tc}}(T_{tc}, \Gamma, \bar{q})$ is given from Eq. (7), when $\phi = T_{tc}$ and $\bar{q} = 1/(\sqrt{2}\beta J)$ which results in $\bar{h}_{T_{tc}} = \sqrt{\sqrt{2}\beta J}\xi$. Furthermore, there is no stable PM solution if

$$\begin{aligned}\mu &< \mu_{at}(T, \Gamma, \bar{q}) && \text{for } T/J > T_{tc}/J, \\ \mu &> \mu_-(T, \Gamma, \bar{q}) && \text{for } T/J < T_{tc}/J.\end{aligned} \quad (10)$$

In Eq. (10), the values of μ_{at} and μ_- are summarized by

$$\mu_\varphi(T, \Gamma, \bar{q}) = \frac{\cosh^{-1}\int D\xi[v_\phi \cosh\sqrt{\Delta_\phi} + u_\phi \sinh\sqrt{\Delta_\phi}]}{\beta}, \quad (11)$$

where

$$v_\phi = \bar{h}_\phi^2/(\bar{q}\bar{\Delta}_\phi) - 1, \quad u_\phi = (\beta\Gamma)^2/(\bar{q}\bar{\Delta}_\phi^{3/2}), \quad (12)$$

with $\bar{\Delta}_\phi$ and $\bar{h}_\phi$ defined in Eq. (9). In Eq. (11), when $\varphi = at$, $\bar{q} = 1/(\sqrt{2}\beta J)$, and when $\varphi = -$, $\bar{q} = [f_\phi(T, \Gamma, \bar{q}) - \sqrt{f_\phi(T, \Gamma, \bar{q}) - 4/(\beta J)^2}]/2$.

In Eq. (10), μ_{at} defines the second order transition line $T_{2f}(\mu)$ and μ_- gives the paramagnetic spinodal line [see Figs. 1(a)-1(h)]. The $\mu_{T_{tc}}$ value is obtained by introducing T_{tc} in equation for μ_{at}.

The PM/SG phase boundary in the T/J-μ/J plane within RS, 1S-RSB Parisi scheme is plotted in Figs. 1(a)-1(d) for $\Gamma = 0$, $0.25J$, $0.5J$, and J, respectively. In Figs. 1(e)-1(h) the position of (T_{tc}, μ_{tc}) (the tricritical point), the first order boundary phase and the spinodal lines are shown in detail. In particular, when $\Gamma = 0$, Fig. 1(a) displays the first order boundary confirming the existence of a reentrance in the FISG model. The turning on of the transverse field Γ [see Figs. 1(b)-1(d)] produces a strong effect on the entire transition line. For instance, the second order part $T_{2f}(\mu)$ is depressed. For $\mu = 0$, this behavior is reminiscent of the one already found in Ref. 17 in which the freezing temperature decreases toward a QCP when $\Gamma \rightarrow \Gamma_c$. It should be remarked that the location of the tricritical point is also decreasing toward zero while Γ is enhanced. Nevertheless, the most important consequence can be seen in the behavior of the first order boundary phase $T_{1f}(\mu)$ [or equivalently $\mu_{1f}(T)$] and, in particular, in the reentrance [see Figs. 1(e)-1(h)]. For $\Gamma = 0.25J$ and $0.5J$, $T_{1f}(\mu)$ and spinodal
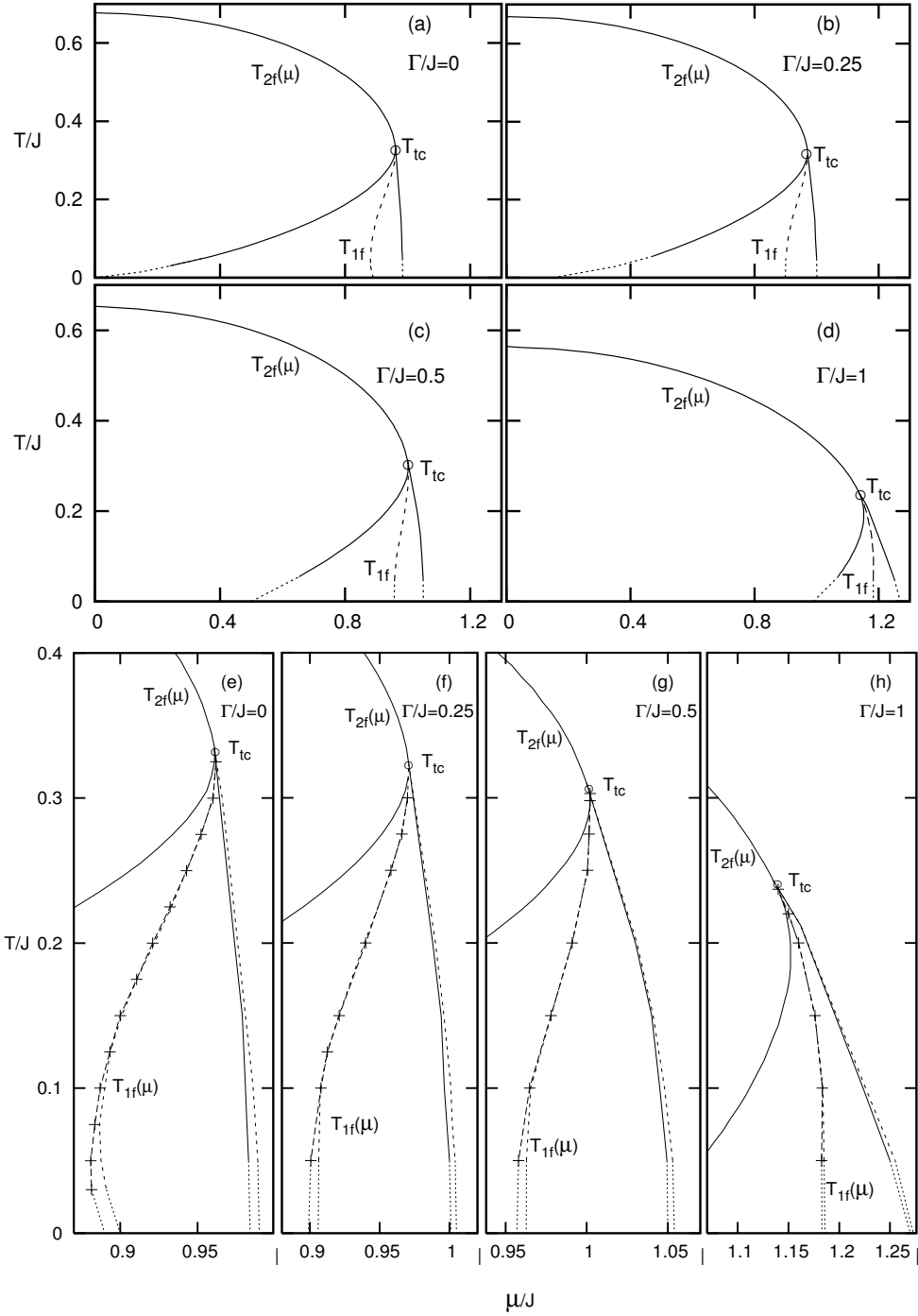
FIG. 1: Panels (a)-(d) show the phase diagrams μ/J versus T/J for several values of Γ/J, where $T_{2f}(\mu)$ indicates the PM/SG second order phase transition, T_{tc} corresponds to the tricritical point, and $T_{1f}(\mu)$ represents the behavior of the first order transition. The spinodal lines are also exhibited (full lines below T_{tc}). Panels (e)-(h) show the first order boundary in detail. In these panels, $T_{1f}(\mu)$ is presented for both the RS (dashed lines) and the 1S-RSB (pointed lines) solutions. They also exhibit the SG spinodal lines for the RS (dashed lines) and 1S-RSB (full lines) solutions. The dotted lines at very low temperatures are extrapolations to $T = 0$.

lines are displaced in order to suppress the reentrance which is completely achieved when $\Gamma = J$. In Fig. 2, the grand canonical potential versus μ/J is plotted at $T = 0.1J$. This figure shows the displacement of first order boundary and spinodal points which illustrate the gradual suppression of the reentrance exhibited in Fig. 1. In Figs. 1 and 2, results are shown within RS and 1S-RSB schemes, which indicate that the location of the first order boundary is weakly dependent on the replica symmetry breaking scheme in agreement with Ref. 4.
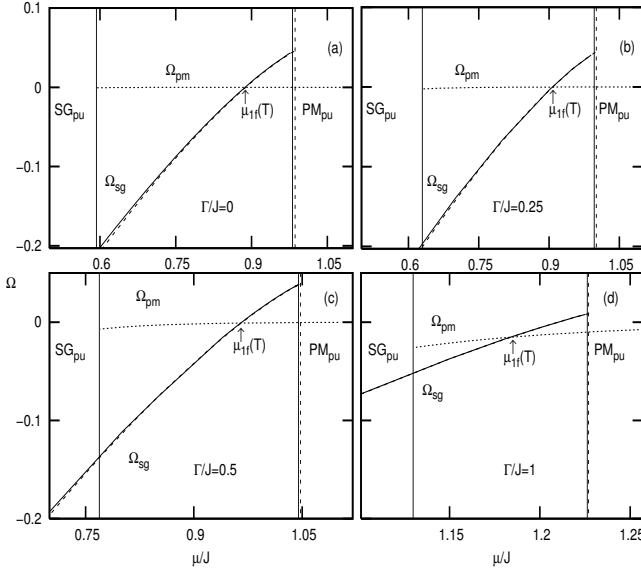
FIG. 2: Grand canonical potential versus μ/J for several values of Γ/J for temperature $T/J = 0.1$. The dotted lines represent the PM canonical potential (Ω_{pm}). The dashed and full lines represent the SG canonical potential (Ω_{sg}) in the RS and 1S-RSB solutions, respectively. The vertical lines are PM (left) and SG (right) spinodal lines. The full vertical line is the 1S-RSB spinodal line. μ_{1f} indicates the first order boundary for $T/J = 0.1$. The labels SG_{pu} and PM_{pu} indicate the regions with only one spin-glass solution and one paramagnetic solution, respectively.

FIG. 3: Entropy versus T/J for several values of Γ/J and μ/J. The first order temperature is equal to $T_{1f}(\mu) = 0.2J$ for all figures. In panels (3a)-(3c), the left vertical lines are the SG spinodal lines and the right vertical lines T_{2f} are the PM/SG second order transitions. At low temperatures ($T/J < 0.2$), in (3a)-(3c), the dashed lines represent the RS spin-glass solution and the dotted lines indicate the 1S-RSB spin glass solution. In panel (3d), the vertical line is the PM spinodal line. The labels SG_{pu} and PM_{pu} indicate the regions with only one SG solution and one PM solution, respectively.

There is some indication the Γ weaken even more such dependence. However, we can not be conclusive on this point due to numerical difficulties, in particular, at low temperature.

In Fig. 3, the entropy versus temperature is show. The values of μ are adjusted to cross the point $T_{1f}(\mu) = 0.2J$ in the first order boundary transition. This procedure allows us to follow the entropy difference between SG and PM phases always at the same point of the first order boundary transition. For $\Gamma = 0$, we can see that the entropy of the PM phase is found below the SG one at the first order transition at $\mu = 0.92J$, which is expected from the existence of inverse freezing in the FISG model as previously discussed.[4] The increase in Γ produces the decrease in the entropy difference between SG and PM phases and the displacement of the first order boundary transition $\mu_{1f}(0.2J)$ to larger values of μ. Simultaneously, the pure PM phase (region PM_{pu} in Fig. 3) is enlarged until the total disappearance of the pure SG phase (region SG_{pu} in Fig. 3). Those effects are related to the suppression of the reentrance shown in Figs. 1 and 2.

The previous results clearly show that the spin flipping, due to the transverse field Γ, suppresses the reentrance in the first order boundary PM/SG transition and, therefore, the inverse freezing. Actually, Γ depresses $T_{2f}(\mu)$ and the tricritical point which also implies that the first
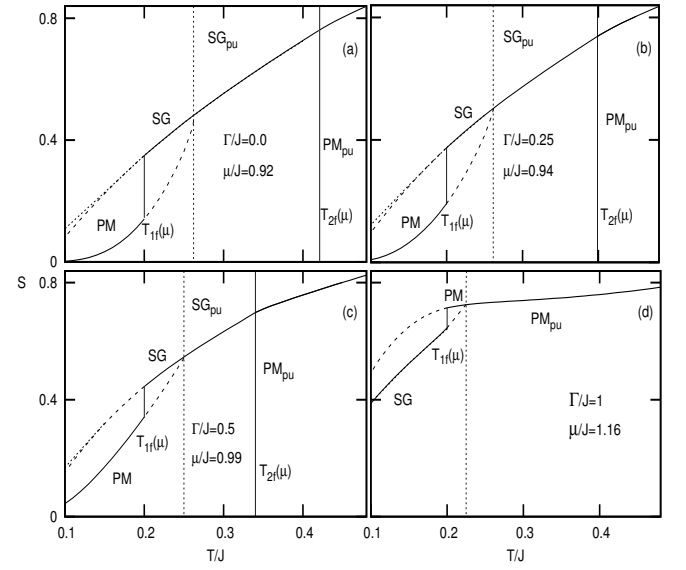
order boundary appears in a decreasing interval of temperature. It is known that, in the FISG model, the average occupation of the nonmagnetic states exponentially decreases with the temperature.[13] Thus, the enhance of Γ would lead the phase transition to exist in a scenario where the nonmagnetic states are unimportant. That scenario is also consistent with the behavior of n as a function of Γ which has been studied by us for several isotherms. In that case, Γ tends to preserve the half-filling occupation even if μ increases. This effect becomes stronger when the temperature decreases. In that sense, the increase in Γ would redistribute charge in such way that the nonmagnetic states become gradually avoided at low temperature. There is no guarantee that the nonmagnetic states in each site have been simply excluded by adjusting n. However, earlier results support such scenario. In Ref. 17, the FISG model has been studied with an additional local restriction to get rid of the nonmagnetic states. The obtained results have shown that, while Γ increases, the transition lines with the restriction and without restriction over the nonmagnetic sites at the half-filling become increasingly close.

To conclude, in the present work, we have studied the role of spin flipping due to Γ in the inverse freezing of the FISG model. It should be remarked that FISG model presents inverse freezing when $\Gamma = 0$ with no need of entropic advantage.[2,4] As main result, it has been shown

that Γ destroys the reentrance in the PM/SG first order boundary and, thus, the inverse freezing. Our results suggest that Γ in the FISG model acts to redistribute the charge occupation, particularly, at low temperature. In that process, the nonmagnetic states become unimportant for the phase transition. In that sense, Γ plays an opposite role concerning the inverse freezing as compared to the degeneracy parameter r of Ref. 2. Although this results are restrict to the FISG model, we can speculate if the suppression of the inverse freezing by the increase in quantum effects can be a more general result.

[*] Electronic address: ggarcia@ccne.ufsm.br

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